Benzoic acid, 3,6-dichloro-2-hydroxy-

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 1.05e-11 cm3/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 2.22e-01

Confidence level: 5.63e-01

Nearest Neighbors from the Training Set

Image not found
1,4-Naphthoquinone
Measured: 3.10e-12
Predicted: 3.16e-11

Image not found
2,5-Furandione
Measured: 1.45e-12
Predicted: 2.17e-12

Image not found
2-Methyl-p-benzoquinone
Measured: 2.35e-11
Predicted: 2.15e-11